ITAPS

INTEROPERABLE TOOLS FOR ADVANCED PETASCALE SIMULATIONS

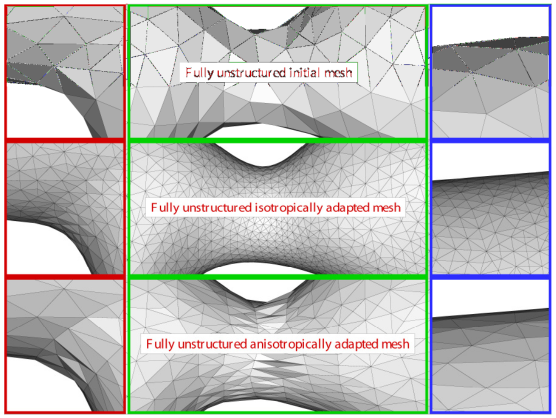
ITAPS Adaptive Mesh Service

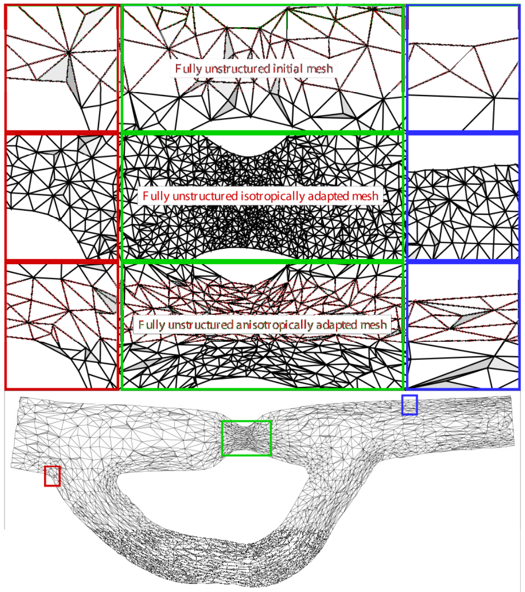
Mark Shephard (RPI)
Ken Jansen (RPI)
RPI SCOREC Team

SciDAC
Scientific Discovery through Advanced Computing

Motivation

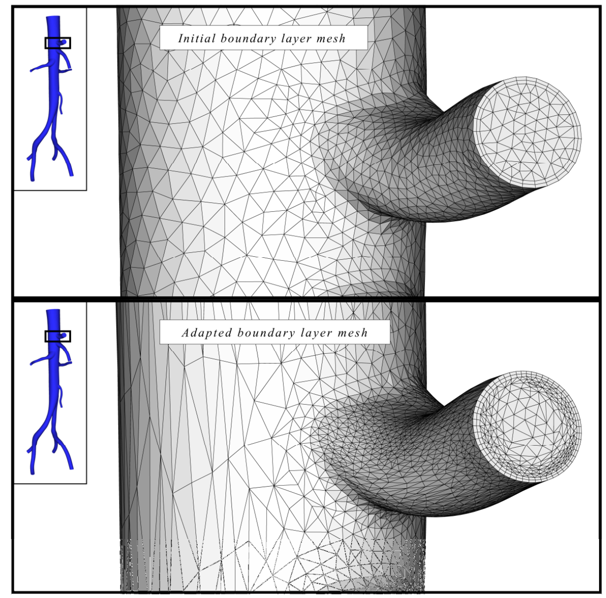
- Complex geometry and/or complex physics generate solutions with large variation in length scales
- Assigning near optimal mesh sizes for initial mesh generation in such cases is not possible
- ITAPS Mesh Adapt Service starts with an arbitrary initial mesh with a solution and alters the mesh via local mesh modifications (may be isotropic or anisotropic)
- CFD example:
  - Isotropic adaptivity yields same accuracy as uniform with one order of magnitude fewer elements
  - Anisotropic adaptivity yields same accuracy as uniform with two orders of magnitude less than uniform

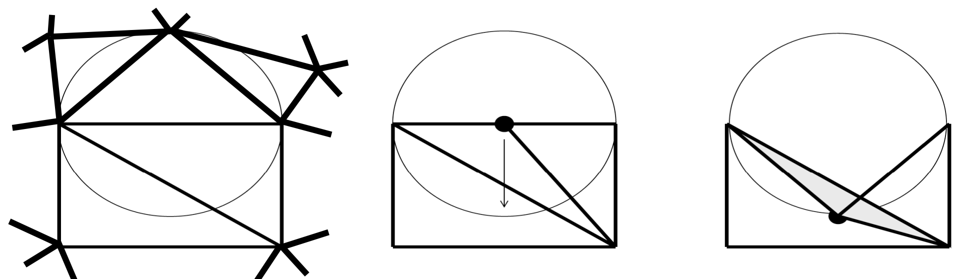




ITAPS Mesh Adapt Service

- Components of an adaptive analysis loop
  - PDE solver
  - Error estimation procedure
  - Mesh adaptation - ITAPS Mesh Adapt Service
  - Field solution transfer - ITAPS Mesh Adapt Service can support
- ITAPS Mesh Adapt Service
  - Input is a mesh and new mesh size field definition: isotropic or anisotropic
  - Mesh adaptation uses local mesh modification to support:
    - Curved Boundaries
    - Anisotropy
    - Parallel mesh adaptation

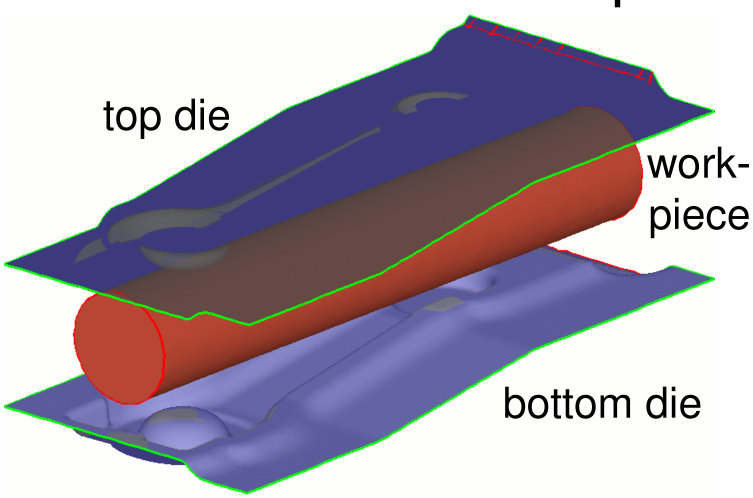


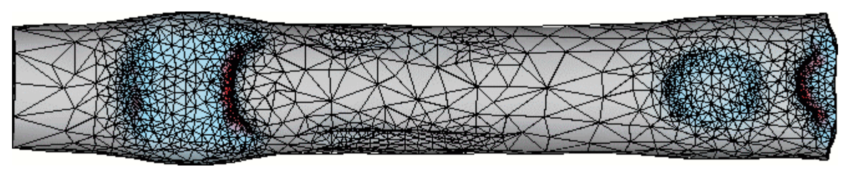


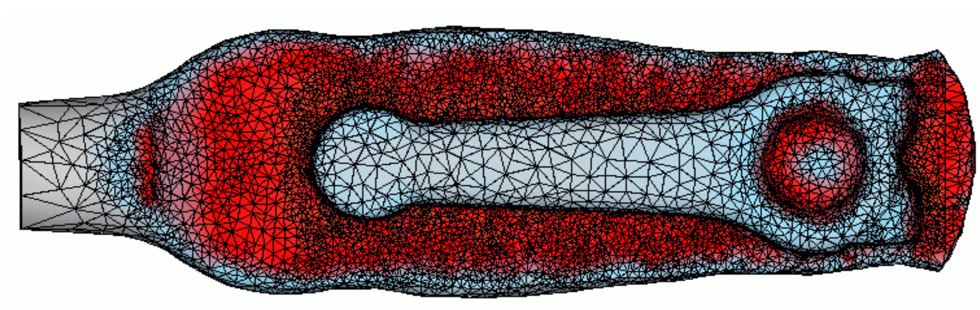
a) b) c)

Example Application: Forming Simulation

- Large plastic deformation - Meshes become invalid
- Components of automated adaptive simulation
  - Model topology update based on contact evolution
  - Mesh adapted using automation tools to account for
    - Discretization errors
    - Geometric approximation
    - Element shape control

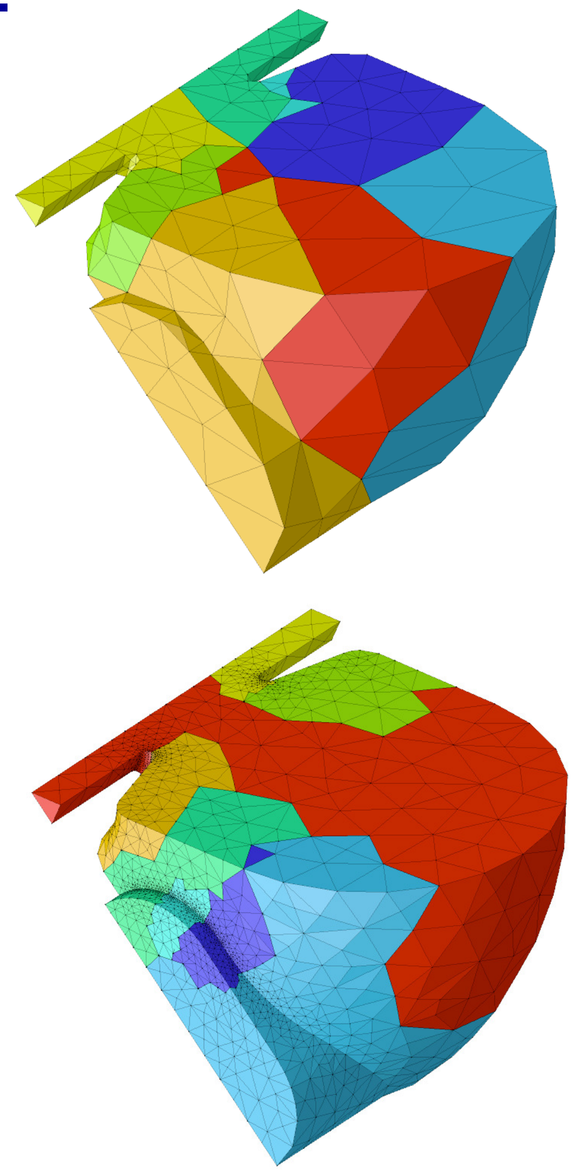






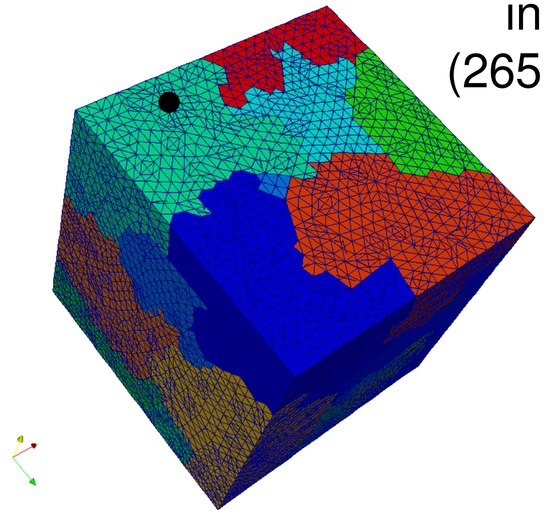
Parallel Mesh Adaptation

- Operates with a partitioned mesh
- Control parallel communication and operations
- Part boundaries do not introduce artificial constraints on execution of mesh modification operations
- By including dynamic load balancing (Zoltan), can be easily integrated with parallel solvers that also operate with partitioned meshes

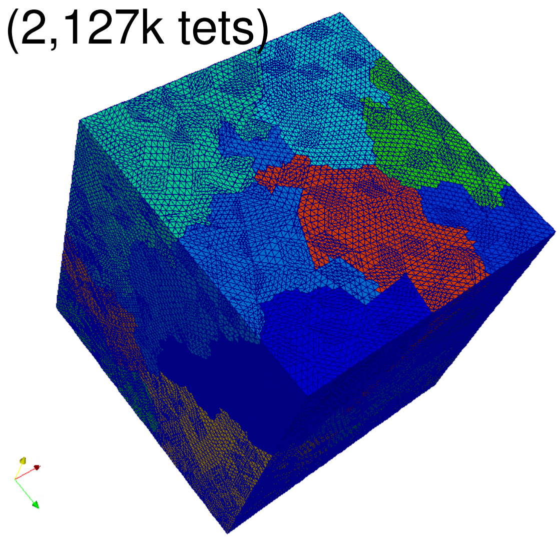


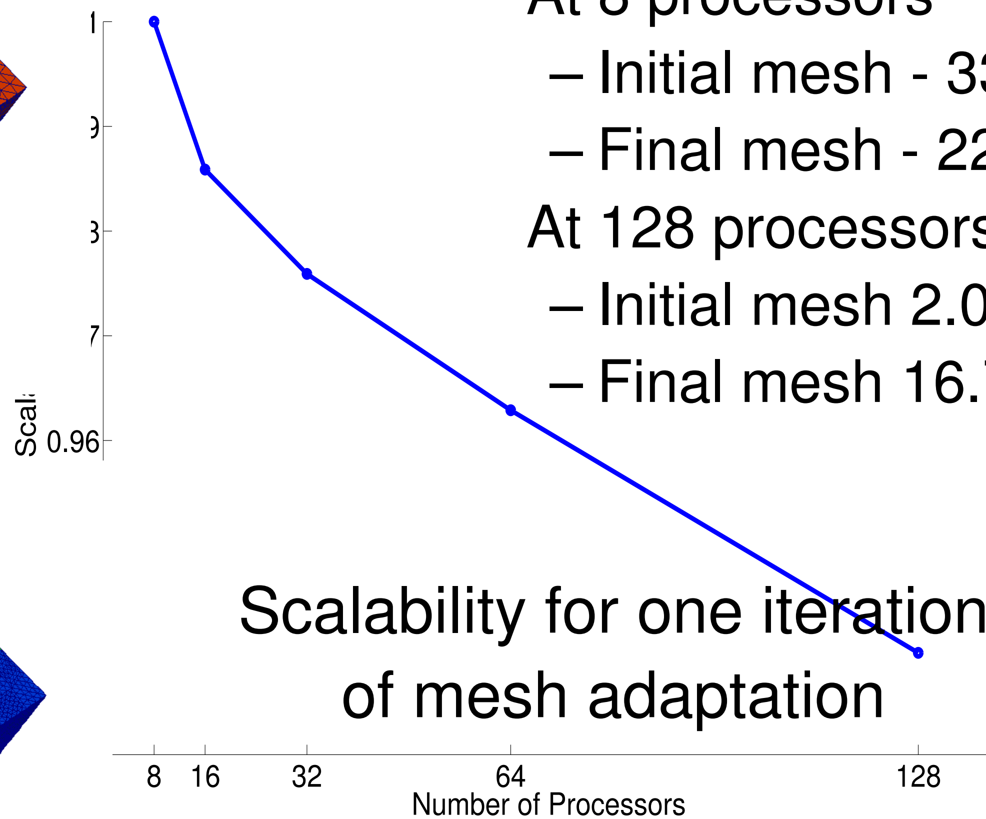
Parallel Refinement

initial
(265k tets)



adapted
(2,127k tets)





Scalability for one iteration of mesh adaptation

Tests run on IBM Blue Gene/L

At 8 processors

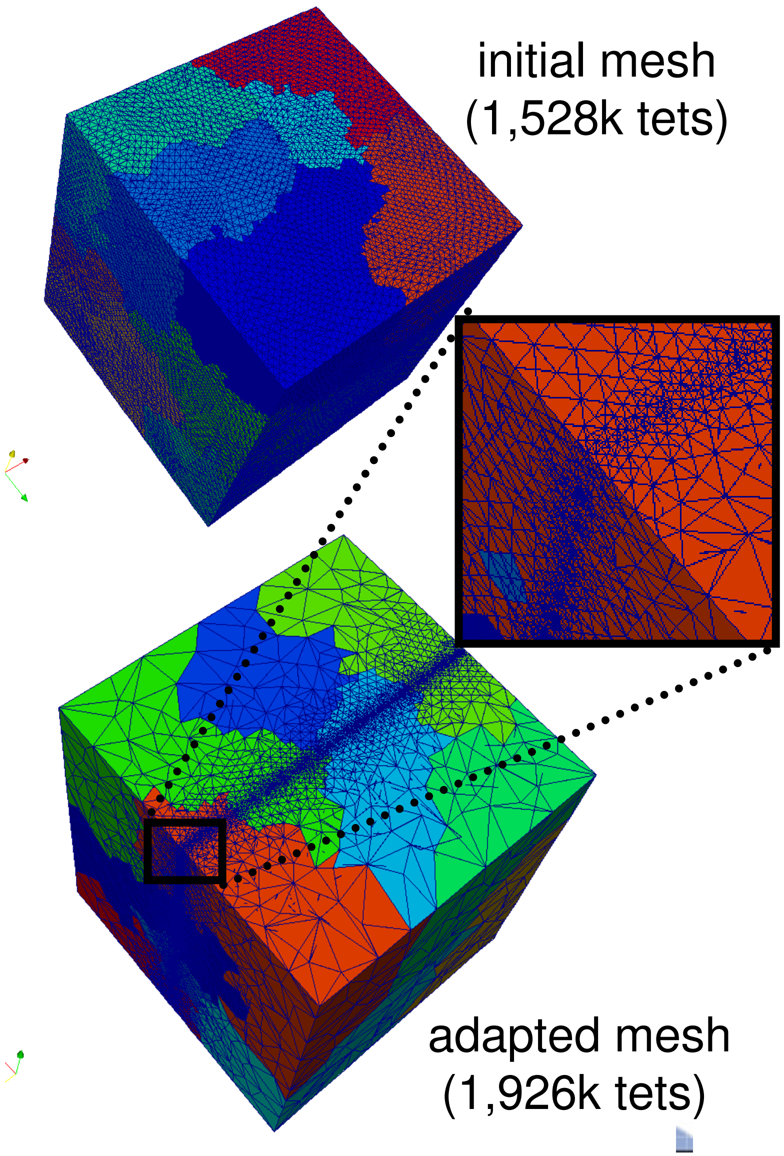
- Initial mesh - 33K/processor
- Final mesh - 226K/processor

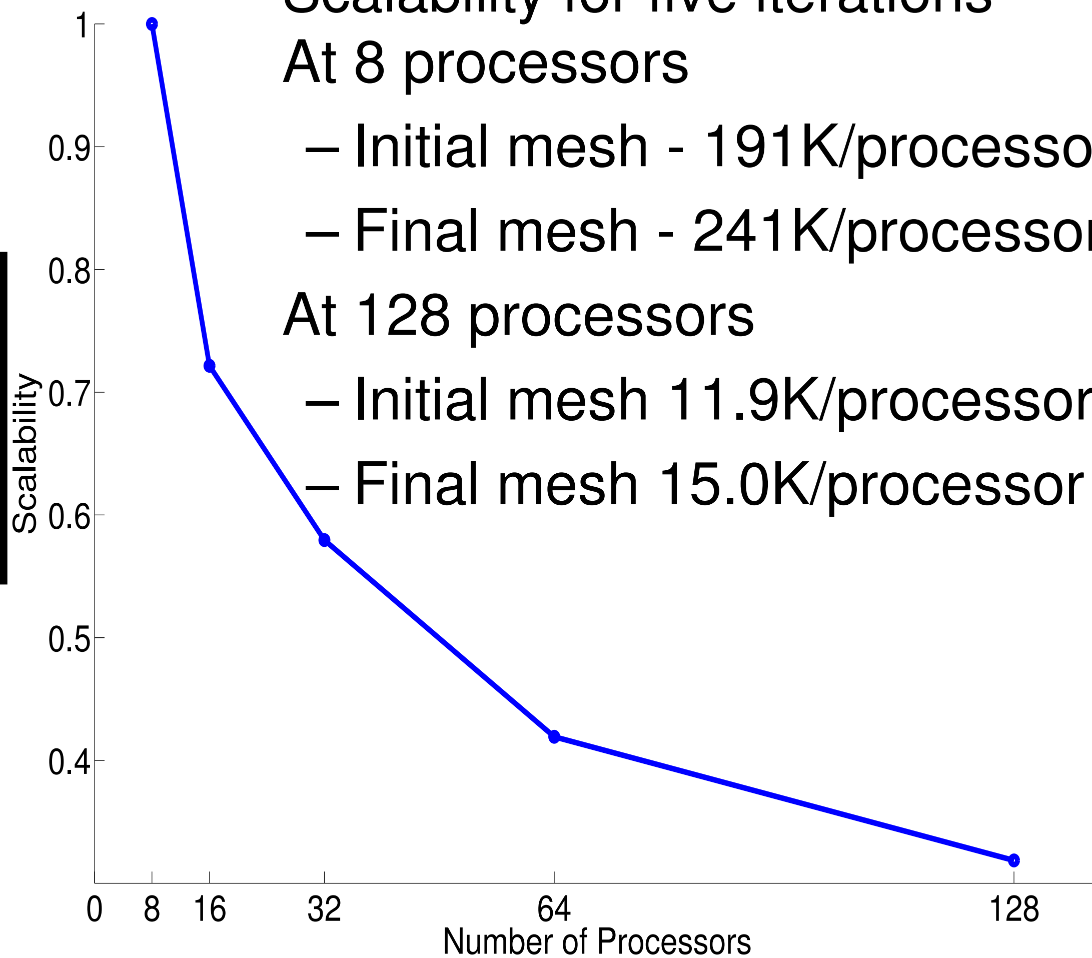
At 128 processors

- Initial mesh 2.0K/processor
- Final mesh 16.7K/processor

$$\text{Scalability} = \frac{\text{run-time}_{\text{base}} \bullet n \text{ processors}_{\text{base}}}{\text{run-time} \bullet n \text{ processors}}$$

Parallel Refinement and Coarsening





Scalability for five iterations

At 8 processors

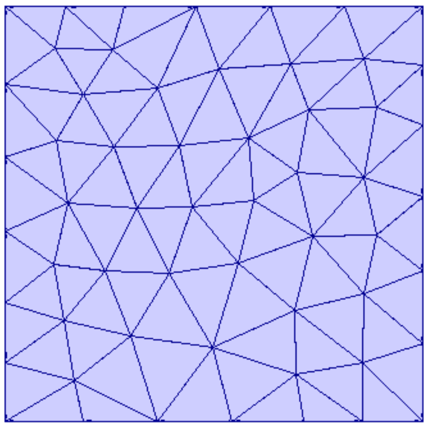
- Initial mesh - 191K/processor
- Final mesh - 241K/processor

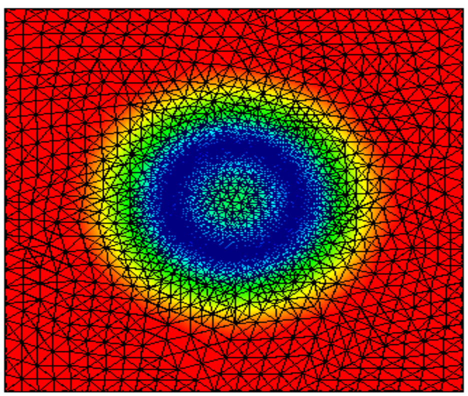
At 128 processors

- Initial mesh 11.9K/processor
- Final mesh 15.0K/processor

$$\text{Scalability} = \frac{\text{run-time}_{\text{base}} \bullet n \text{ processors}_{\text{base}}}{\text{run-time} \bullet n \text{ processors}}$$

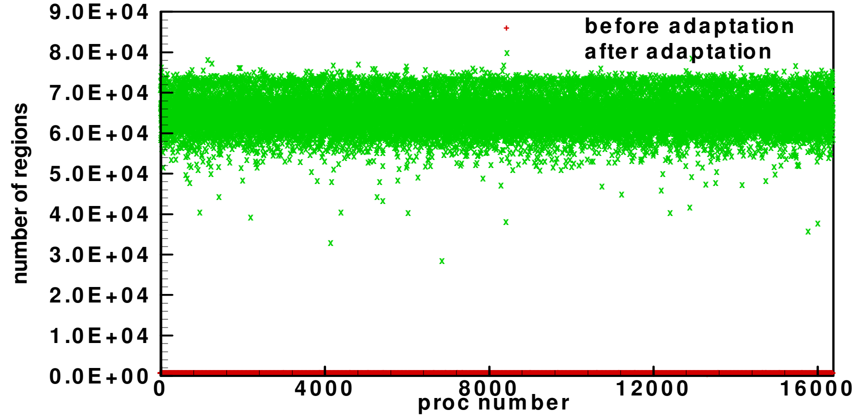
Mesh Adaptation for 1 Billion Element Mesh





Initial and adapted mesh at one bubble - colored by magnitude of mesh size field

Mesh size field of air bubbles distributing in a tube (segment of the model)



Number of regions of adapted mesh among 16k parts

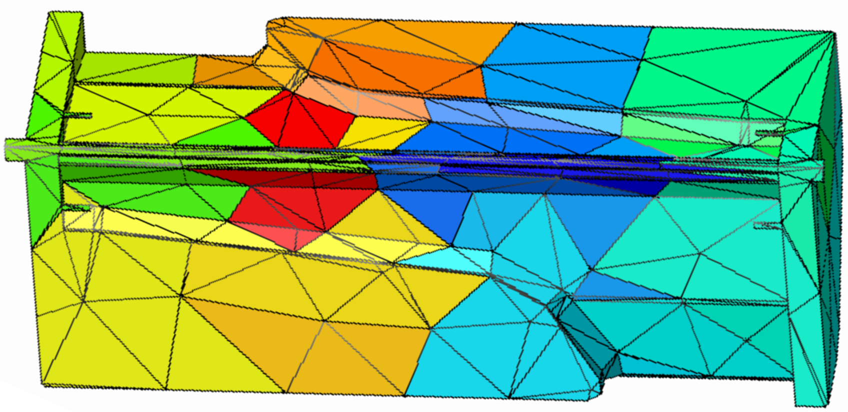
- Initial mesh: uniform, 17,179,836 mesh regions
- Adapted mesh: 160 air bubbles 1,064,284,042 mesh regions
- Multiple predictive load balance are used to make the adaptation possible
- Larger meshes possible (not out of memory) but this element count is appropriate for solver

Parallel Adaptive Applications

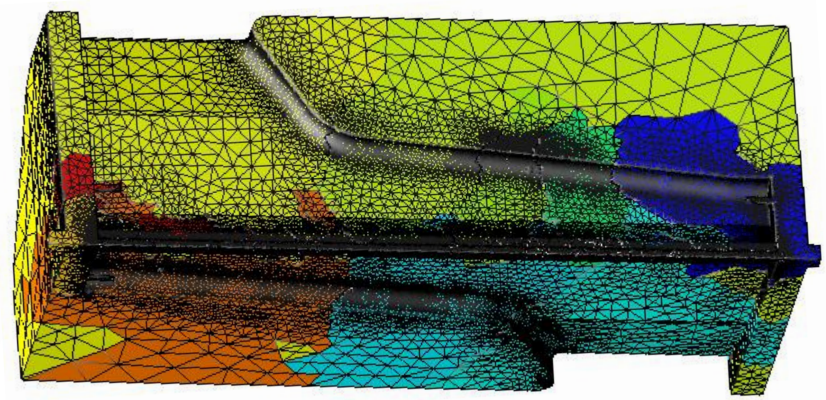
- Parallel adaptive application requires integration of parallel components for
  - Unstructured grid solver
  - Error estimation and mesh size field construction
  - Mesh adaptation
  - Dynamic load balancing with repartitioning
- With these components ITAPS has constructed parallel adaptive applications

Adaptive Loop for SLAC Accelerator Design

– Components:
  - ACIS CAD modeler, Omega3P
  - ITAPS/SCOREC mesh adaptation
  - Error estimations
– Parallel adaptive loop control



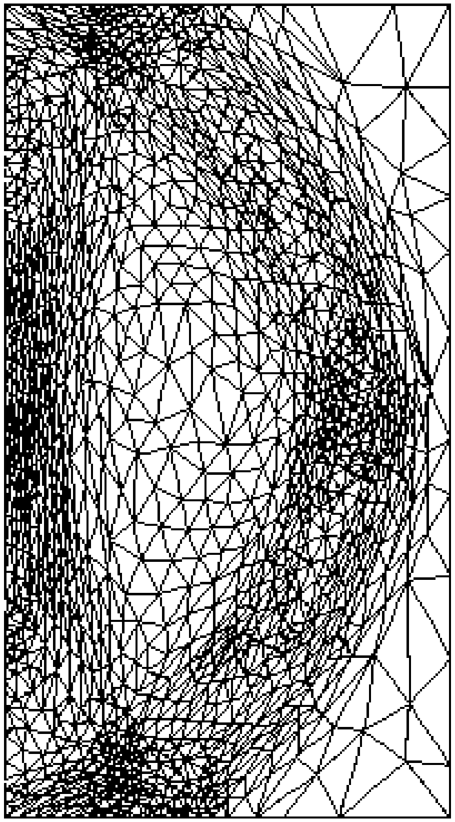
Initial mesh (1,595 tets)

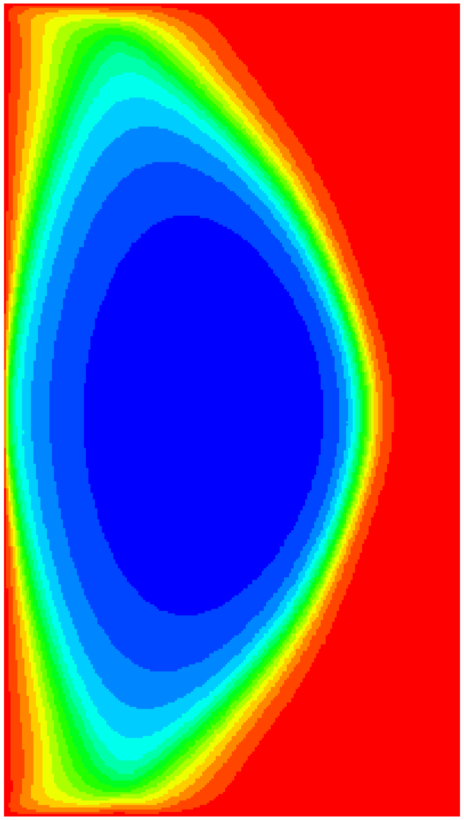


Adapted mesh (23,082,517 tets)

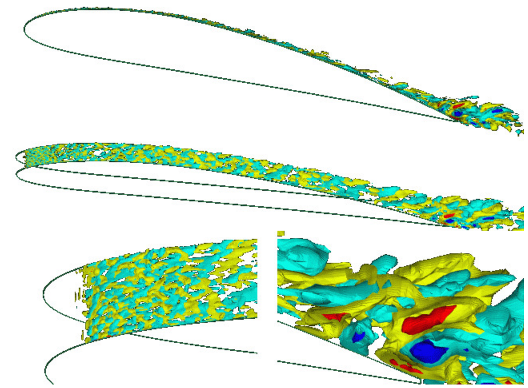
Adaptive Loop for PPPL CEMM M3D-C1 MHD Simulations

- Restructured M3D-C1 to support general unstructured meshes
- Provided API level for interacting with mesh and solvers (three-way interactions between CEMM, ITAPS and TOPS)
- Developed initial anisotropic mesh adaptation procedure
- Extending code to deal with complex boundary conditions on curved domains using the high order M3D-C1 elements

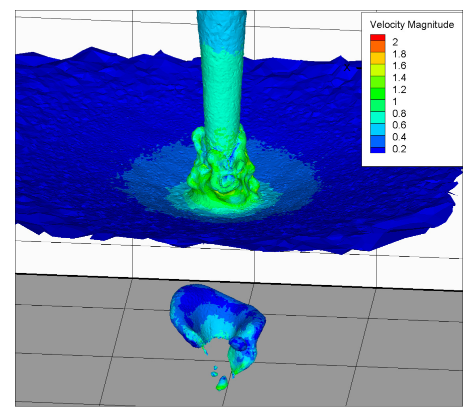




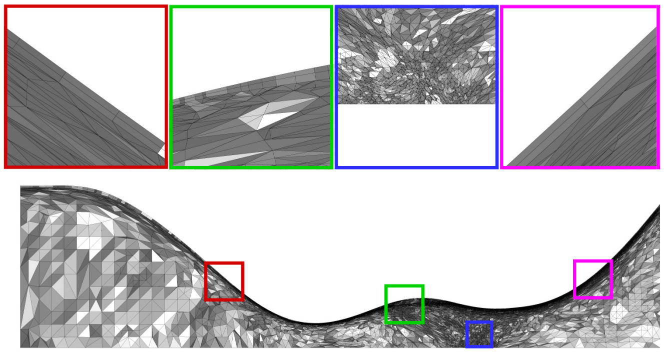
PHASTA Flow Simulation Code

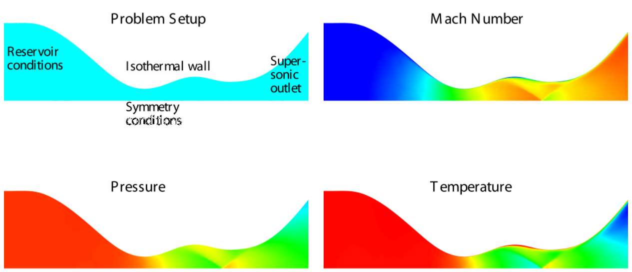


- Parallel finite element flow solver
  - compressible and incompressible flows
  - Turbulence DNS, LES, RANSS/DES
  - Two-phase (immiscible) fluids
- Implicit time integration -
  - solution of linear algebra at each time step using iterative solvers
- Breaks the total domain into parts with roughly the same number of elements on each processor.
- Work can be characterized as requiring:
  - Substantial floating point operations to form equations
  - Organized, substantial, and regular communication between partitions that touch each other
  - For each iteration (O(10) iterations per solve), there is a required ALL-REDUCE communication



Strong scalability results for double-throat nozzle (1.5M elems.)





Cores (avg. elems./core)	BigBen, PSC (Cray XT3)		Ranger, TACC (Sun Constellation)		CCNI-BG/L, RPI (IBM's BlueGene/L)	
	t (secs.)	scale factor	t (secs.)	scale factor	t (secs.)	scale factor
16 (96000) - base	390.84	**1** (base)	425.96	**1** (base)	2121.10	**1** (base)
32 (48000)	190.63	**1.03**	208.73	**1.02**	1052.42	**1.01**
64 (24000)	89.57	**1.09**	98.10	**1.09**	528.62	**1.00**
128 (12000)	46.08	**1.06**	50.05	**1.06**	265.37	**1.00**
256 (6000)	24.49	**1.00**	27.70	**0.96**	132.83	**1.00**
512 (3000)	13.28	0.92	14.81	0.90	67.35	**0.98**
1024 (1500)	7.97	0.77	9.63	0.69	33.70	**0.98**
2048 (750)	-	-	-	-	17.13	**0.97**
4096 (375)	-	-	-	-	9.09	0.91
8192 (187)	-	-	-	-	5.00	0.83

scale factor, $s_i = (t_{base} \times np_{base}) / (t_i \times np_i)$
1 implies perfect scaling

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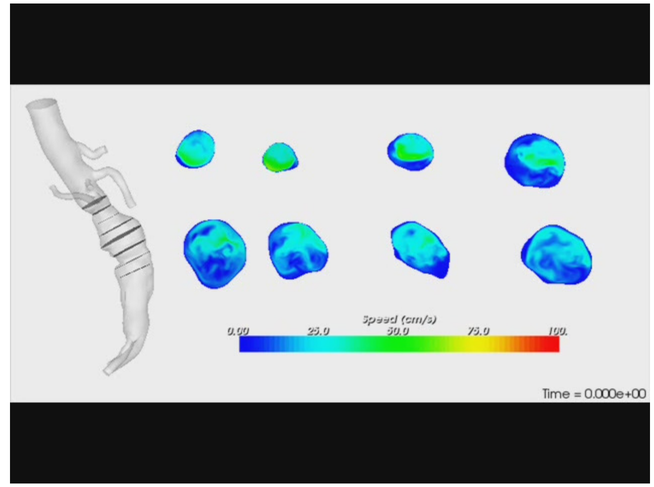
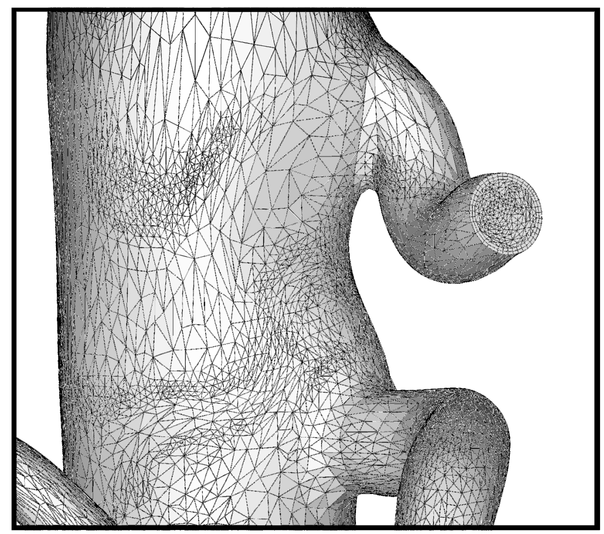
Strong scalability results for abnormal aortic aneurysm (105M elems.):

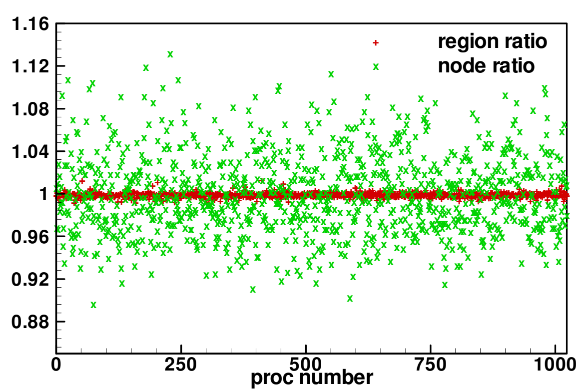
Cores (avg. elems./core)	CCNI-BG/L, RPI (IBM's BlueGene/L)	
	t (secs.)	scale factor
512 (204800)	2119.7	**1** (base)
1024 (102400)	1052.4	**1.01**
2048 (51200)	529.1	**1.00**
4096 (25600)	267.0	**0.99**
8192 (12800)	130.5	**1.02**
16384 (6400)	64.5	**1.03**
32768 (3200)	35.6	0.93





32K parts show modest degradation due to 15% node imbalance (with only about 600 mesh-nodes/part)

Rgn./elem. ratio$_i$ = rgns$_i$/avg_rgns
Node ratio$_i$ = nodes$_i$/avg_nodes



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Strong scalability: abdominal aortic aneurysm (~ 105M elems.)

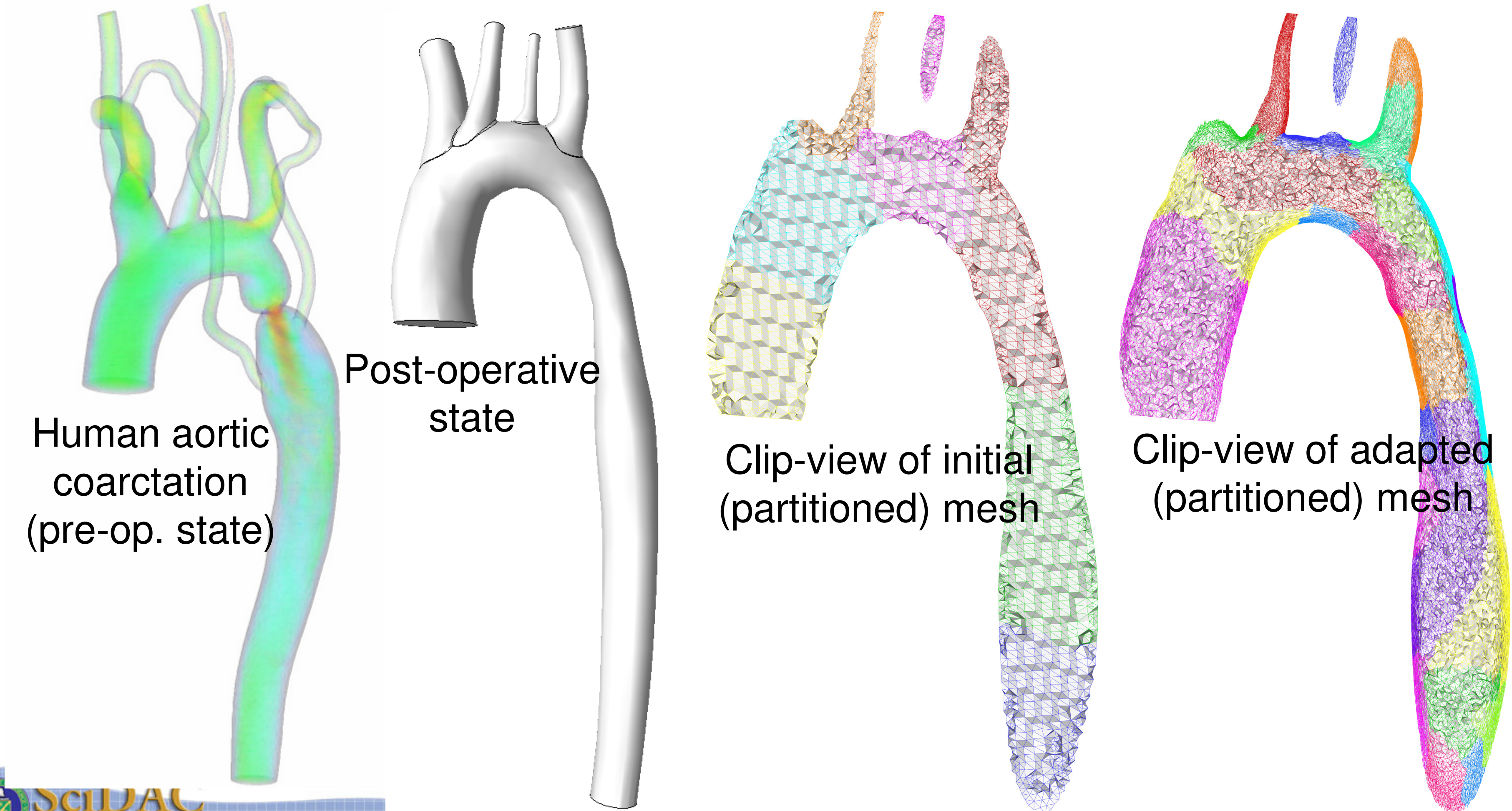
Cores (*avg. elems./core*)	**BigBen, PSC (Cray XT3)**		**Franklin, NERSC (Cray XT4)**		**Ranger, TACC (Sun/Opteron Cluster)**	
	t (secs.)	scale factor	t (secs.)	scale factor	t (secs.)	scale factor
1024 (*102,400*)	406.94	**1** (base)	340.68	**1** (base)	527.87	**1** (base)
2048 (*51,200*)	162.94	**1.25**	151.50	**1.12**	257.82	**1.02**
4096 (*25,600*)	84.04	**1.21**	87.76	**0.97**	156.80	0.84

Detailed studies show a CPU noise problem on Ranger

- CPU noise caused by demons on full systems
- Ranger team have made changes to reduce noise
- Note reduced kernels on cores can avoid this problem (one of the reasons for good Blue Gene results

Evaluating post-operative flow state in human aortic coarctation

(10M elems. in 32 parts, colors indicate different parts in mesh partition)



Human aortic coarctation (pre-op. state)

Post-operative state

Clip-view of initial (partitioned) mesh

Clip-view of adapted (partitioned) mesh

Coupled flow and Wall Deformation

- Fully coupled membrane model requires no mesh motion to capture vessel wall wave propagation at very small additional cost (Figueroa)

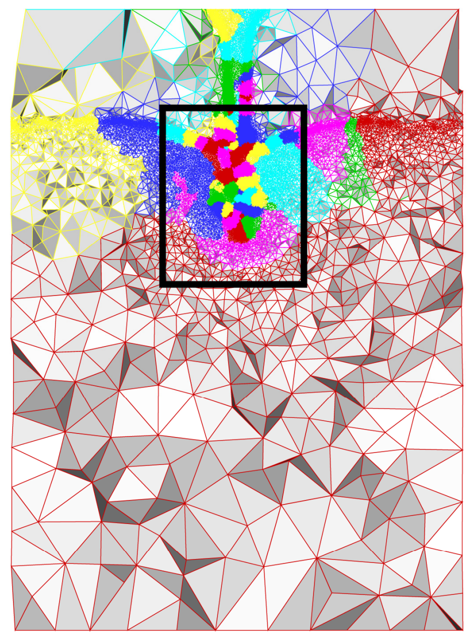
QuickTime™ and a
Microsoft Video 1 decompressor
are needed to see this picture.

Simulating air entrapment in case of plunging jet (two phase with level sets)

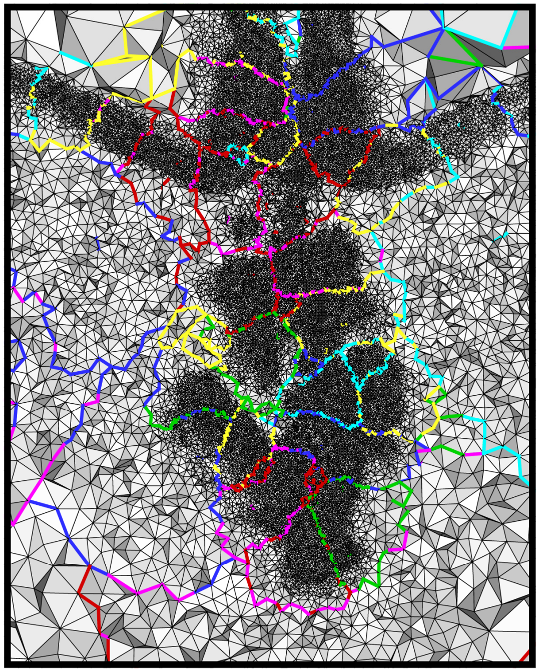
13M elems. in 128 parts, colors indicate different parts

Air entrapped in plunging jet

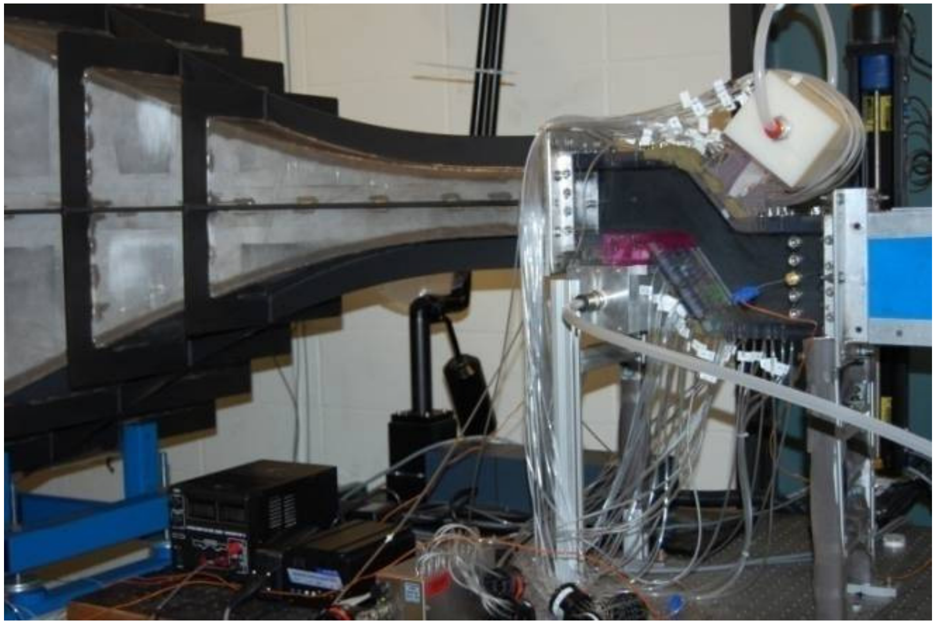
Clip-view of adapted (partitioned) mesh

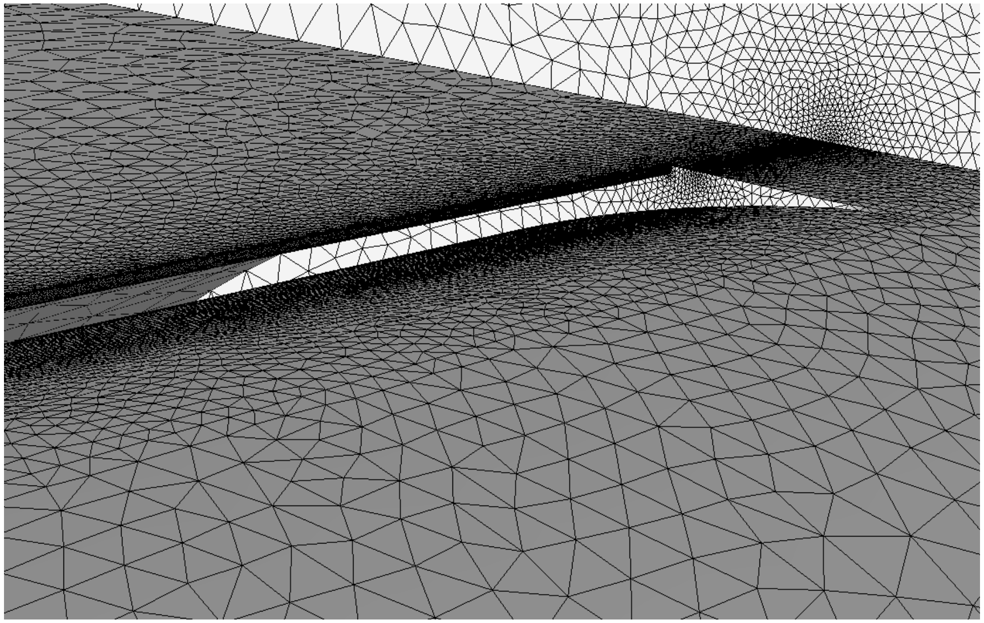


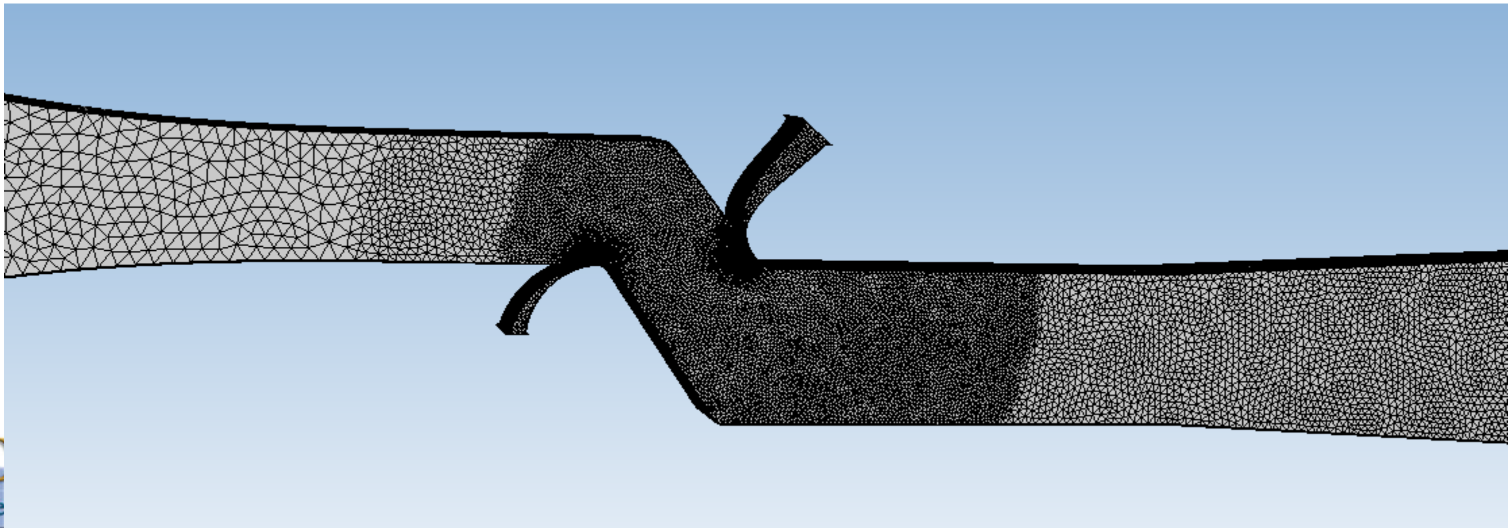
Magnified view of mesh (near air entrapment)



Flow Control: Experiment/CFD/Controls *Amitay & Wen*







CFD: RANSS Results